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THEORETICAL TRAJECTORIES OF CHARGED PARTICLES IN AN INHOMOGENEOUS MAGNETIC FIELD

by

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ABSTRACT

This theoretical study of the trajectories of charged particles supplements an experimental project of molecular-ionic rearrangements using the magnetic focusing properties of a beta-ray spectrometer. The experimentally measured magnetic field was analytically represented by a twelfth-order polynomial. This field is axially symmetric, but non-homogeneous otherwise. The particular particle of concern was the hydrogen ion, H_2^+. The trajectory of this particle was computed from a second-order differential equation, assuming values for the kinetic energy and initial angle of the particle, and the magnetizing current. The solution was obtained by numerical integration using a CDC 1604 digital computer. The distinctive feature of these calculations, in contrast to those used normally for a beta-ray spectrometer, is the large scattering (initial) angle, about 45°.

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LIST OF ILLUSTRATIONS

TABLE OF SYMBOLS

A	The vector potential
B	The magnetic flux density of the field
B(i)	The coefficients computed for the polynomial which describes the magnetic field on-axis
E	The kinetic energy of the rebound particle, a function of the scattering angle
E_o	The energy of the incident particle
Fi, Gi	Functions of z which are described later in detail
$H_o(z)$	The axial component of the field on axis
H^i	The i-th derivative of the function $H_o(z)$
I_B	The magnetization current
$k = p/q$	
L	The intercept distance measured on the z-axis
ϕ	The azimuthal angle in cylindrical coordinates
p	The momentum of the rebound particle (H_2^+)
q	The magnitude of the electronic charge
r	The radial distance in cylindrical coordinates
θ	The scattering angle measured in the laboratory frame
z	The axial distance in cylindrical coordinates

1. Introduction

This presentation is part of an experimental project presently being conducted at the U. S. Naval Postgraduate School to verify a classical theory developed by Bates, Cook, and Smith [1] of the capture of a light ion or atom from a target system by a fast projectile.

Specifically, the theory involves a reaction of the type:

$$H^+ + CH_4 \rightarrow H^+H + CH_3$$

and is essentially a sequence of binary collisions. The process ensues with the bombardment of methane gas by low energy protons, whereby the resulting rebound proton and escaping hydrogen ion join to form the product H_2^+. The angle of departure (or scatter) is shown to be in the vicinity of 45 degrees, and is labeled θ.

Since the expected cross section will be quite low ($\leq 10^{-18}$ cm^2), a detector could not be utilized, as is standard procedure, by placement at the scattering angle. [5]

Therefore, the beta-ray spectrometer was chosen due to its property which will cause all H_2^+ ions of the same departure angle and energy to converge. This study determines that point of convergence, or focus.

2. Discussion

It is known from elementary electromegnetic theory that a magnetic force, $q\{\vec{v} \times \vec{B}\}$, is produced on a charged particle moving at an angle to the direction of the field. This force causes the particle to sustain a change in velocity (direction only). The supposition is, for this field, that a particle which begins its motion on the axis of the field and at an angle with that field axis, will travel a curvilinear path and ultimately intersect the axis of the field for appropriate values of the field strength, energy and initial angle of the particle. This can be readily shown for a homogeneous field.

The point at which the particle returns to the axis is called the intercept point, and the distance from the origin of the trajectory to the intercept point is the intercept distance (L). This is where the

detector can be placed to analyze the particulate beam. The experimental usefulness is that if the intercept distance is known along with the field strength, and the energy of beam E_o, then the initial angle may be evaluated.

The theoretical problem, which is herein shown, is the evaluation of the intercept distance assuming values for the scattering angle.

Thus, the following intermediate problems arose:

A. A means to express the field, or more precisely, a continuous function which would represent the field for all points in the area of interest.

B. A set of equations to specify the motion of the particle to incorporate the energy and charge of the particle, as well as the interaction of the magnetic field.

C. A numerical method to solve a differential equation which would result from the equations in (B) above.

D. Interpretation and extrapolation from sets of trajectories to obtain these derivatives:

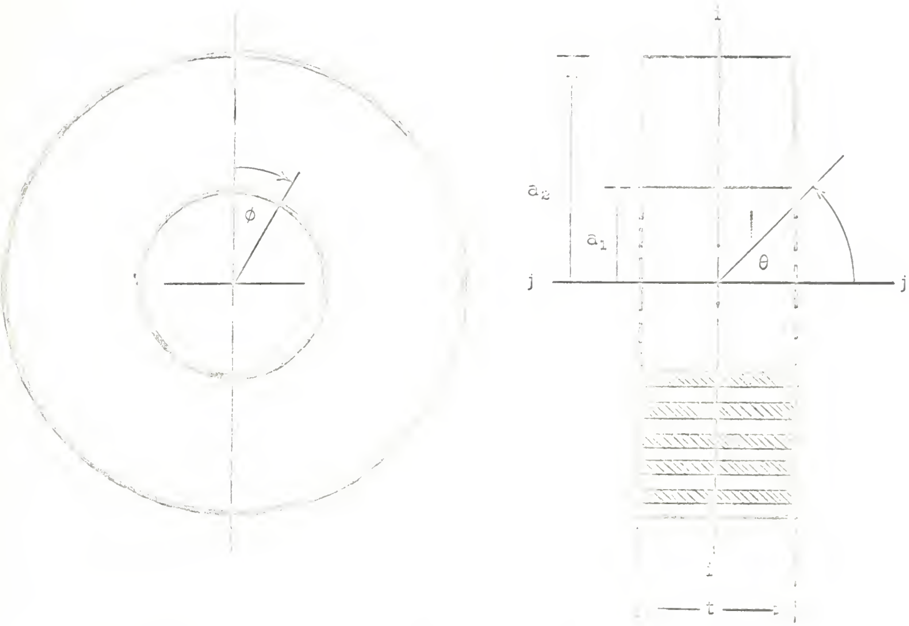
$\left(\frac{\partial L}{\partial E}\right)_{\theta,\, I_B}$ -- The change in intercept distance with respect to changes in energy

$\left(\frac{\partial L}{\partial \theta}\right)_{I_B,\, E_o}$ -- The change in intercept distance with respect to changes in angle

$\left(\frac{\partial L}{\partial I_B}\right)_{E_o,\, \theta}$ -- The change in intercept distance with respect to changes in magnetization current

3. The Magnet and its Field

The magnet which will be used for this project was previously in the USNPGS beta-ray spectrometer. It is essentially composed of a normal section of a right circular cylinder, and wound with cylindrically concentric layers of copper wire. The outer disks and cylindrical center section which form the container for the layers of wire are copper as are the cooling water tubes. The figure (Fig. 1) on the next page shows the magnet with its dimensions.



Blank layers indicate water cooling tubes
Cross-hatched layers, copper wire

a_1 = Inside radius of the coil = 10.17 cm.

a_2 = Outside radius of the coil = 27.30 cm.

t = Thickness of the coil = 15.[illegible]8 cm.

Fig. 1. The Magnet

The experimental field strength of this magnet on-axis, H_0, appears as a Gaussian curve as shown in Fig. 2. The quantities in Appendix 1 for the values of the field are shown in the positive z direction. The maximum intensity of the field on-axis is at the geometrical center of the magnet, at the point formed by the intersection of lines ii and jj. B has cylindrical symmetry about the line jj, and is symmetrical about the center plane.

In order to more easily discuss the field, the system of cylindrical coordinates should be established at this point. The origin is defined to be at the intersection of the lines ii and jj. The line jj will be the z axis, and the radial distance, r, will be measured perpendicularly from it. The angular component, ϕ, is as in (r, ϕ, z), a right hand coordinate system.

Measurements were made on this field for various values of field current by P. J. Kelly in May 1965 with an axial Hall Probe, and this data has been compiled in Appendix 1. The axial component of the field intensity was measured initially on the primary axis of the magnet (z axis) for a distance of 66 cm. on either side of the origin at 4 cm. intervals. This was done for various current settings between 2 and 14 amperes.

Also, the axial component of the field was measured off axis at four values of z, and for 8 values of ϕ, for each value of z. The radius r was varied from zero to seven cm.

The conclusions concerning the field were that:

(1) The field strength is linear with current over the entire range of current settings within an accuracy of ±0.1%.

(2) The field is symmetrical on either side of the $z = 0$ plane to ±0.01%.

(3) The field is azimuthally symmetric to ±0.01%.

To find the analytic expression for the field on axis, $H_0(z)$, where z assumes positive values only, a polynomial was fit to the data by the method of least-squares. This data is contained in Appendix 1. A

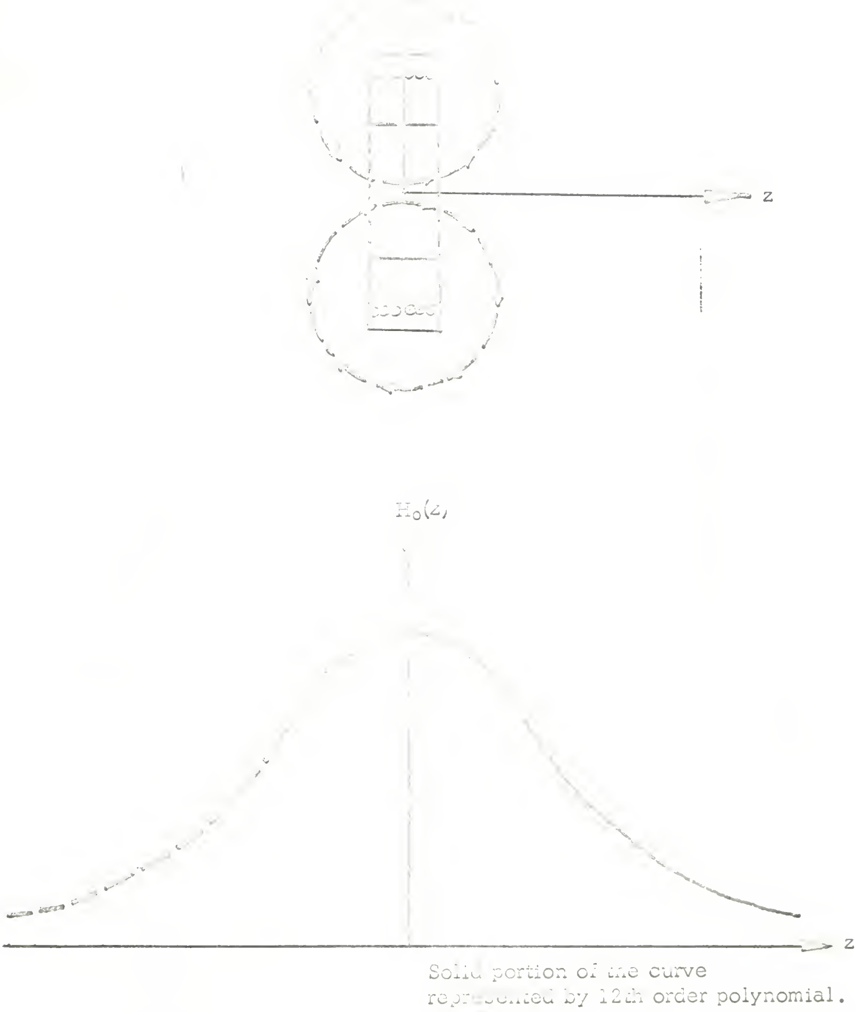


Fig. 2. The Magnetic Field

twelfth order polynomial was chosen, and provided sufficient precision in the form:

$$H_0(z) = B_1 + B_2 z + B_3 z^2 + B_4 z^3 + B_5 z^4 + \ldots + B_{13} z^{12} \quad . \qquad (3\text{-}1)$$

The thirteen coefficients were determined by the computer and a USNPGS subroutine LSQPOL, which is in PROGRAM CURVE included in Appendix 6.

At this point, a comparison was made of the experimental field values and those values which would result from the polynomial field expression.

To make this check of the values of the field off-axis, the following steps were taken:

(1) The vector potential was computed for all values of r and z using the derived polynomial.

(2) The axial component of the field was derived, using the vector potential, and evaluated for various values of r and z.

This computation is shown in detail in Appendix 1. The agreement between experimental and theoretical values was again quite good.

4. Theory of the Trajectory

The H_2^+ ion has a positive charge equal in magnitude to that of the electron, and mass essentially equal to twice the mass of a single proton. The mass of the single electron is ignored.

The path of this particle can be represented by this equation:

$$\left[\frac{r''}{1 + (r')^2}\right]\{k^2 - A^2\} - r'(A)\left[\frac{\partial A}{\partial z}\right] + A\left[\frac{\partial A}{\partial r}\right] = 0 \qquad (4\text{-}1)$$

where A is the vector potential, and k is defined as (mv/q). The prime above indicate differentiation with respect to z. A discussion of A, its derivatives, and k will follow.

This equation for any charged particle can be derived from the equations of motion for that particle which begins its path on the primary axis of the magnetic field. This equation is derived in Appendix 4.

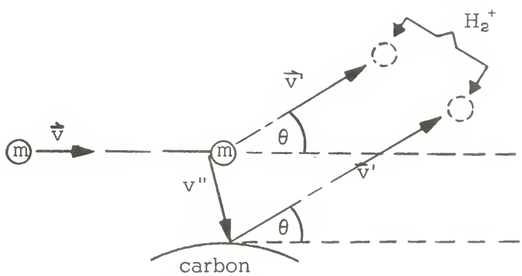
The energy of the H_2^+ particle after scattering is E, and can be shown to be:

$$E = 2\,E_0\,\cos^2\,\theta \qquad (4\text{-}2)$$

where E_0 is the kinetic energy of the particle which is incident on the target methane. The angle θ is again the angle of scatter.

A description of the collision process is as follows:
The incoming proton strikes one of the hydrogens in the methane molecule. This is the first of the two binary collisions, and the only one which is assumed to be totally elastic. The initial particle moves off at an angle, called the departure angle; and the second particle (essentially a proton and an electron) moves towards the carbon atom at an angle equal to $90^\circ - \theta$. Since the carbon atom is assumed to be infinitely massive, compared to the hydrogen atom approaching it, this second particle is redirected in the second binary collision in the direction of the recoiling proton.

A schematic of the collision process is as follows:



In the laboratory frame, the initial energy of the system is:

$$E_0 = \tfrac{1}{2}\,m_1\,(\vec{v}_1)^2 \qquad (4\text{-}3)$$

and the final energy is:

$$E = \tfrac{1}{2}\,(2m)(\vec{v}')^2 \qquad (4\text{-}4)$$

Conservation of momentum yields, for the first collision:

$$P_x = m\vec{v} = m\vec{v}'\cos\theta + m\vec{v}''\sin\theta \qquad (4\text{-}5)$$

and,

$$p_y \quad = m\vec{v}' \sin\theta - m\vec{v}'' \cos\theta = 0 \qquad (4\text{-}6)$$

The last equation results in

$$\vec{v}'' = \vec{v}' \tan\theta \qquad (4\text{-}7)$$

and substituting into the equation (4-5)

$$\vec{v}' = \vec{v} \cos\theta\ . \qquad (4\text{-}8)$$

With this relationship between the velocities, the final energy after the two collisions becomes

$$\begin{aligned} E &= \tfrac{1}{2}(2m)\ (\vec{v}')^2 \qquad (4\text{-}4) \\ &= \tfrac{1}{2}(2m)\ v^2 \cos^2\theta \\ &= 2E_0 \cos^2\theta \end{aligned}$$

$$E = 2E_0 \cos^2\theta \qquad (4\text{-}2)$$

If both collisions are elastic in nature, then it is quite easy to show that θ must be 45°. The y-component of momentum produces the equation

$$p_y \quad = m\vec{v}' \sin\theta - m\vec{v}' \cos\theta = 0 \qquad (4\text{-}9)$$

at the first collision. And it can only be satisfied when

$$\sin\theta = \cos\theta$$

or, when $\theta = 45^\circ$.

5. Expression for the Vector Potential

The fact that the field is cylindrically symmetric carries with it the implication that there is no azimuthal component, since the curl B = zero. This field can be described by a vector potential which is always in the azimuthal direction.

Using the calculated expression for magnetic field on-axis, $H_0(z)$, the vector potential expansion

$$A(r,z) = \frac{r}{2} H_0(z) - \frac{r^3}{16}\left(\frac{\partial}{\partial z}\right)^2 H_0(z) + \frac{r^5}{384}\left(\frac{\partial}{\partial z}\right)^4 H_0(z) \qquad (5\text{-}1)$$

$$+ \dots + \frac{(-1)^n}{n!\ (n+1)!}\left(\frac{r}{2}\right)^{2n+1}\left(\frac{\partial}{\partial z}\right)^{2n} H_0(z) + \dots$$

is shown to be for any point (r,z):

$$A = \frac{r}{2}[G_1] - \frac{r^3}{16}[G_2] + \frac{r^5}{384}[G_3] - \frac{r^7}{18432}[G_4] + \frac{r^9}{1474560}[G_5]$$

$$- \frac{r^{11}}{176947200}[G_6] + \frac{r^{13}}{29727129600}[G_7]$$

where $\left(\frac{\partial}{\partial z}\right)^n H_0(z)$ is the nth partial derivative of the function $H_0(z)$ with respect to z, and where $G_1 = H_0(z)$, and $G_2 = \left(\frac{\partial}{\partial z}\right)^2 H_0(z)$, etc.

6. The Computer Solution

It remains, at this point, to find the solution of the differential equation. The method chosen for this task was a process of numerical integration employing a digital computer. The subroutine INTEG-1 of the USNPGS Computer Library was selected because of its adaptability to this particular problem. The program in which INTEG-1 is contained is called PROGRAM ORBITS, and is listed as Program C in Appendix 6.

The first four statements of this program (ORBITS) are standard according to the instructions for use of INTEG-1. The three comment cards that follow describe ENER, OKAY, and P, which are names given various quantities used in the solution.

B(1) through B(13) are the coefficients used in the polynomial as obtained by PROGRAM CURVE. The functions F(1) through F(6), and G(1) through G(7) are explained in Appendix 5.

VECDZ is the symbol for the partial derivative of the vector potential with respect to z. VECDR represents the partial derivative of the vector potential with respect to r. VECPT is the vector potential.

A second order differential equation can be reduced to a system of two first differential equations. Applying this technique to equation (4-1) yields

$$[r']' = r' \frac{[A \frac{\partial A}{\partial z}]}{[k^2 - A^2]} + (r')^3 \frac{[A \frac{\partial A}{\partial z}]}{[k^2 - A^2]} - (r')^2 \frac{[A \frac{\partial A}{\partial r}]}{[k^2 - A^2]} - \frac{[A \frac{\partial A}{\partial r}]}{[k^2 - A^2]} \tag{6-1}$$

$$[r]'' = r' \qquad (6\text{-}2)$$

Letting

$$x(1) \equiv r \qquad \text{and} \quad x(2) \equiv r' ,$$

the equations (6-1) and (6-2) become

$$[x(2)]' = [x(2)]\,\mathrm{FUNC4} + [x(2)]^3\,\mathrm{FUNC4} - [x(2)]^2\,\mathrm{FUNC5} - \mathrm{FUNC5}$$

$$[x(1)]' = x(2)$$

where

$$\mathrm{FUNC4} = \frac{[A \frac{\partial A}{\partial z}]}{[k^2 - A^2]}$$

$$\mathrm{FUNC5} = \frac{[A \frac{\partial A}{\partial r}]}{[k^2 - A^2]}.$$

Further, FUNC4 and FUNC5 can be written in terms of FUNC1, FUNC2 and FUNC3 as follows:

$$\mathrm{FUNC1} = k^2 - A^2$$

$$\mathrm{FUNC2} = A \frac{\partial A}{\partial z}$$

$$\mathrm{FUNC3} = A \frac{\partial A}{\partial r}$$

and

$$\mathrm{FUNC4} = \frac{\mathrm{FUNC2}}{\mathrm{FUNC1}}$$

$$\mathrm{FUNC5} = \frac{\mathrm{FUNC3}}{\mathrm{FUNC1}}$$

OKAY is obtained in the following way. This is the machine language expression for k^2 where the energy can be entered in eV. In the MKS system, k must have the unit of webers/meter. This is the same as A, since B has the units of webers/meter^2, and $\vec{B} = \nabla \times \vec{A}$.

$$k = \frac{m\,v}{q} \quad \text{in units of} \quad \frac{(\text{kilogram})(\text{meter/sec})}{(\text{coulombs})} \quad \text{or webers/meter.}$$

It would be desirable to have k expressed in terms of the energy of the particle, E, and in the units of eV, as a great savings in conversion would be realized.

Using the non-relativistic expression for the energy E, the following is obtained:

$$E = \frac{p^2}{2m} \qquad \therefore\ p = (2mE)^{\frac{1}{2}}$$

But, since k^2 is needed

$$k^2 = \frac{p^2}{q^2} = \frac{2mE}{q^2} = \frac{2mE'}{q} \qquad \text{if } E' \text{ is expressed in eV.}$$

And, k^2 becomes

$$\left[\frac{2(\text{mass of } H_2^+)}{\text{charge of electron}}\right] E'$$

Inserting the values of the constants, k^2 becomes the quantity OKAY:

$$\text{OKAY} = \left\{\frac{4(1.6725 \times 10^{-27}}{1.6021 \times 10^{-19}}\right\} E'$$

$$= \{4.17576 \times 10^{-8}\} E'$$

or

OKAY = (4.17576E - 08)*(ENER), as expressed in the program.

The method of solution employed by INTEG-1 is a fourth order Runge-Kutta numerical integration approximation of the ordinary differential equations.

The computation is performed in the MKS system of units.

TO USE PROGRAM ORBITS (the main trajectory program)

This program is written in the language of FORTRAN-60. Its successful employment depends on the correct use of the data cards, which are the last eight cards of the program itself. These eight cards contain the input information, and the quantities desired as output. An example of the data cards may be seen on the last page of Program C in Appendix 6.

Data card #1: This card is used for identification, and columns 2-32 are available for this use. This title appears on all data output, as well as graphs.

Data card #2: This card contains the number of "runs", or trajectories, to be processed with a maximum of 9. This number is entered in column 1 of the card. Note, however, that only one graph is possible for the entire program.

Data card #3: The number of coupled first-order differential equations is specified by this card (maximum of 30). In this case, there are two and this number is posted, right justified, in columns 1 and 2, as 02.

Data card #4: The initial and final values of the independent variable, z, over which the integration process is to be carried out. The integration step size is also stipulated. The integration can be processed in up to 3 segments, each with a different step size, thus:

$$ZI \xrightarrow{S1} Z1 \xrightarrow{S2} Z2 \xrightarrow{S3} ZF,$$

or $ZI \xrightarrow{S1} Z1 \xrightarrow{S2} ZF$,

or $ZI \xrightarrow{S1} ZF$,

where ZI refers to the initial value of z (in this case equal to zero), ZF refers to the final value of z, Zi refers to intermediate values of z, and Si are the step sizes. All of these numbers are entered in meters. The corresponding values, with decimal points, are placed in the above order in columns 1-10, 11-20, 21-30, etc.

Data card #5: Columns 1-10 contain the value of the energy E in electron-volts, again, with the decimal point. Columns 11-20 contain the quantity P which adjusts the magnetic field according to

the base of 10 amperes magnetization current. For example, for a field of 7 amps, the quantity 0.70 would be entered anywhere in columns 11-20.

Data card #6: Here are the values of the initial conditions. The format is the same as for cards 4 and 5. The first value expressed is the initial value of r (equal to zero), and the next value is the slope of the function at that point, $\left(\frac{dr}{dz}\right)$. This derivative may be considered to be also the tangent of the scattering angle, θ.

Data card #7: This card controls data print-out. A blank card will suppress this output. Again, using the ten column sequence, this format is as follows. The first 8 columns contain the title for each variable output desired, and the last two columns contain the variable identifier. The variable identifiers are 00 for z, 01 for r, and 02 for r'. An example: Z DIST 00R DIST 01SLOPE 02

Data card #8: This last data card controls graph output. A blank card will suppress this output. Remember: that only ONE graph for each submitted program can be drawn and it corresponds to the first set of data. The information is contained in columns 1-20. Columns 1-16 contain the graph title, and columns 17-20 indicate the variable identifiers. Columns 17-20 must always be 0100. The origin, direction of plot, and scale distances have already been set within the main program.

Running Time: The time required for the computer solution is dependent on the step size and the total range of the independent variable. This running time has averaged about three minutes for a single trajectory.

7. Results

The outcome of this project was the creation of a single-package system which generates hydrogen ion trajectories in an axially symmetric field.

Approximately 100 production trajectories were computed for values of energy E ranging from 97 eV to 450 eV; magnetizing current from 7 to 15 amperes; and scattering angle of 35-55 degrees. The

numerical output data and the graph plots showed these orbit configurations to be quite smoothly continuous and consistent.

The error in evaluating the intercept distance L was due mainly in the uncertainty of reading the graph or interpolating the data printout. These values of L ranged from 20 centimeters to about 80 centimeters, with an estimated error of $\pm 1.0\%$. The maximum radial distance of the orbits was around 8 cm.

Comparison of these computer trajectories with those obtained by the fine wire technique used by Kelly showed only fair agreement to within $\pm 10.0\%$. The disparities in the different sets of trajectories have not as yet been determined.

This computer system was checked with a constant uniform (homogeneous) magnetic field against an analytic solution. The comparative results were excellent (to within $\pm 0.01\%$).

Based on a Standard Trajectory of $E_o = 300$ eV,

I_B = Magnet current = 12 amperes,

$\theta = 45$ degrees:

$$\left.\frac{\partial L}{\partial \theta}\right)_{E_o,\, I_B} = -3.3 \pm 0.2 \text{ cm/deg}$$

$$\left.\frac{\partial L}{\partial I_B}\right)_{\theta,\, E_o} = -9.7 \pm 0.8 \text{ cm/amp}$$

$$\left.\frac{\partial L}{\partial E_o}\right)_{I_B,\, \theta} = 0.20 \pm 0.01 \text{ cm/eV}$$

The above derivatives show that as θ and I_B are increased, L is decreased. However, an increase in E_o produces an increase in L. Each of the partial derivatives were obtained with respect to a change in a single parameter, with the other two parameters held constant.

8. Acknowledgements

In this limited space and manner, I note with pleasure all those people from whom I have received impetus towards the completion of this study. To them, I render my personal appreciation.

I wish to thank Professors F. D. Faulkner and H. M. Martinez of the Department of Mathematics, Professors F. W. Terman and J. R. Ward of the Electrical Engineering Department, and Professors O. Heinz and R. L. Armstead of the Physics Department for their inspiration, encouragement and assistance.

Prof. Ward provided invaluable assistance and advice as to the modification of the integration and draw systems of the main trajectory program. Prof. Heinz, at whose suggestion and under whose guidance the central project is being undertaken, contributed his ideas and enthusiasm. Prof. Armstead, as my thesis advisor, aided with his timely counsel, helpful suggestions and continued confidence; and to him, I am sincerely indebted.

To all the personnel of the Computer Facility, USNPGS, and, in particular, Mrs. Robin Ekstrum, I salute for their extreme consideration. Without their cooperation, the task would have been manyfold more difficult.

Finally, I am grateful to my wife, Dorothy, for her understanding and devotion throughout this undertaking, and for typing the draft copy.

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APPENDIX 1

DATA ON THE MAGNETIC FIELD

The magnet which provides this inhomogeneous field was formerly employed in the beta-ray spectrometer which was reconstructed here at the USNPGS in the period 1955-56. Although much was known about the magnet itself, there existed no data on the magnetic field until measurements were made by Kelly [5] in 1965.

This data has been compiled and is herein available for the field strength both on- and off-axis; and also, for the theoretically computed as well as experimentally measured values in Gauss.

In the diagram of the Magnetic Field Strength in this appendix, there are two values listed for each (r, z). The experimental values in the diagram are the upper ones listed in each square.

The theoretically computed values are listed in squares and are the lower values. The method by which these values were computed is as follows:

The field on-axis is given by:

$$H_0(z) = B_1 + B_2 z + B_3 z^2 + B_4 z^3 + B_5 z^4 + \ldots + B_{13} z^{12} \qquad (3\text{-}1)$$

(z expressed in meters)

where:

B(1) = 8.0498907E-02
B(2) = 2.3351831E-02
B(3) = -4.8664438E+00
B(4) = 4.2887590E+01
B(5) = -4.3626183E+02
B(6) = 3.9271101E+03
B(7) = -2.2648265E+04
B(8) = 8.2393030E+04
B(9) = -1.9359723E+05
B(10) = 2.9437706E+05
B(11) = -2.8025472E+05
B(12) = 1.5200646E+05
B(13) = -3.5865075E+04

Since A_ϕ is the only non-zero component of the vector potential, the axial component of the field strength, H_z , can be computed and compared to values obtained by the Hall Probe.

H_z becomes $\frac{1}{r}\left\{\frac{\partial}{\partial r}\left([r \; A_\phi]\right)\right\}$

where A_ϕ is equation (5-1).

And, after performing the indicated operations,

$$H_z \; (r,z) = G_1 - \frac{r^2}{4} G_2 + \frac{r^4}{64} G_3 - \frac{r^6}{2304} G_4 + \ldots. \qquad (11)$$

This is demonstrated in Appendix 6.

r \ z	0.0	2.	6.	10.	14.	18.	22.	26.	30.	34.	38.	42.	46.	50.
7.62	892 904				395 399							61 61		
6.35	864 881				407 408							61 62		
5.08	840 858				413 416							61 63		
3.81	821 837				420 421							61 63		
2.54	810 820				423 424							63 64		
1.27	804 808				425 427							63 64		
0.00	803 804	793 793	702 701	566 566	427 427	313 313	231 230	172 172	131 130	100 100	80 79	63 64	53 52	43 43

MAGNETIC FIELD STRENGTH (in Gauss)
All distances on axes in centimeters

Upper values - experimental
Lower values - theoretical

APPENDIX 2

USEFUL FORMULAE IN CYLINDRICAL COORDINATES

Conversion from Rectangular Coordinates:

$$x = r\cos\phi$$
$$y = r\sin\phi$$
$$z = z$$

The Gradient

$$\vec{\nabla}\Phi = \left(\frac{\partial\Phi}{\partial r}\right)\hat{r} + \frac{1}{r}\left(\frac{\partial\Phi}{\partial\phi}\right)\hat{\phi} + \left(\frac{\partial\Phi}{\partial z}\right)\hat{k}$$

The Divergence

$$\vec{\nabla}\cdot\vec{A} = \frac{1}{r}\left\{\frac{\partial(rAr)}{\partial r}\right\} + \frac{1}{r}\left\{\frac{\partial A\phi}{\partial\phi}\right\} + \left\{\frac{\partial Az}{\partial z}\right\}$$

The Curl

$$\vec{\nabla}\times\vec{A} = \frac{1}{r}\left[\frac{\partial Az}{\partial\phi} - \frac{\partial(rA\phi)}{\partial z}\right]\hat{r} - \left[\frac{\partial Az}{\partial r} - \frac{\partial Ar}{\partial z}\right]\hat{\phi} + \frac{1}{r}\left[\frac{\partial(rA\phi)}{\partial r} - \frac{\partial Ar}{\partial\phi}\right]\hat{k}$$

The Laplacian

$$\nabla^2\Phi = \frac{1}{r}\left\{\frac{\partial}{\partial r}\left(r\frac{\partial\Phi}{\partial r}\right)\right\} + \frac{1}{r^2}\left\{\frac{\partial^2\Phi}{\partial\phi^2}\right\} + \left\{\frac{\partial^2\Phi}{\partial z^2}\right\}$$

APPENDIX 3

POWER SERIES EXPANSION TO OBTAIN THE VECTOR POTENTIAL

The well known expansion, equation (5-1) will now be derived. This expression describes the vector potential for an inhomogeneous magnetic field, which acts only in the azimuthal direction. The field on-axis, $H_o(z)$, and its even derivatives can be computed.

Basically, the derivation of this expansion is as follows: Since the field is constant and involves no currents in the region of the field,

$$\vec{\nabla} \times \vec{B} = 0.$$

And,

$$\vec{B} = \vec{\nabla} \times \vec{A},$$

so that the vector equation for which a solution is desired is:

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{A}) = 0.$$

Conditions for this field are:

$$B_\phi = 0,$$

and $A_r = A_z = 0.$

In cylindrical coordinates, $\nabla \times B$ becomes

$$\vec{\nabla} \times \vec{B} = \frac{1}{r}\left[\frac{\partial B_z}{\partial \phi} - \frac{\partial (rB_\phi)}{\partial z}\right]\hat{r} - \left[\frac{\partial B_z}{\partial r} - \frac{\partial B_r}{\partial z}\right]\hat{\phi} + \frac{1}{r}\left[\frac{\partial (rB_\phi)}{\partial r} - \frac{\partial B_r}{\partial \phi}\right]\hat{z},$$

and each component must be equal to zero.

$$\frac{\partial B_z}{\partial r} = \frac{\partial B_r}{\partial z} \tag{1}$$

$$B_r = \frac{1}{r}\left[\frac{\partial A_z}{\partial \phi}\right] - \left[\frac{\partial (rA_\phi)}{\partial z}\right] = \frac{1}{r}\left\{-\frac{\partial (rA_\phi)}{\partial z}\right\} \tag{2}$$

$$B_\phi = \frac{\partial A_z}{\partial r} - \frac{\partial A_r}{\partial z} \equiv 0$$

$$B_z = \frac{1}{r}\left[\frac{\partial (rA_\phi)}{\partial r}\right] - \frac{\partial A_r}{\partial \phi} = \frac{1}{r}\left\{\frac{\partial (rA_\phi)}{\partial r}\right\} \tag{3}$$

From equations 1, 2 and 3,

$$\frac{\partial}{\partial r}\left[\frac{1}{r}\left\{\frac{\partial}{\partial r}(rA)\right\}\right] = -\frac{\partial}{\partial z}\left[\frac{1}{r}\left\{-\frac{\partial}{\partial z}(rA)\right\}\right] \quad \text{, and}$$

$$\frac{\partial}{\partial r}\left[\frac{1}{r}\left\{r\frac{\partial A}{\partial r} + A\right\}\right] + \frac{\partial}{\partial z}\left[\frac{1}{r}\left\{\frac{\partial r}{\partial z}A + r\frac{\partial A}{\partial z}\right\}\right] = 0, \text{ and}$$

$$\frac{\partial}{\partial r}\left[\frac{\partial A}{\partial r} + \frac{A}{r}\right] + \frac{\partial}{\partial z}\left[\frac{\partial r}{\partial z}\frac{A}{r} + \frac{\partial A}{\partial z}\right] = 0,$$

and the partial derivative $\frac{\partial r}{\partial z}$ is zero as the coordinates are independent.

Thus,

$$\frac{\partial^2 A}{\partial r^2} + \frac{1}{r}\frac{\partial A}{\partial r} - \frac{A}{r^2} + \frac{\partial^2 A}{\partial z^2} = 0.$$

Here, a solution is assumed in the form $\sum_{n=0}^{\infty} a_n(z)\, r^n$ where the coefficients $a_n(z)$ are differentiable. To determine the coefficients,

$$\frac{\partial A}{\partial r} = \Sigma\, n\, a_n(z)\, r^{n-1},$$

and

$$\frac{\partial^2 A}{\partial r^2} = \Sigma\, n(n-1)a_n(z)\, r^{n-2},$$

and

$$\frac{\partial A}{\partial z} = \Sigma\, a_n'(z) r^n,$$

and

$$\frac{\partial^2 A}{\partial z^2} = \Sigma\, a_n''(z)\, r^n$$

Substituting in, and multiplying through by r^2

$$\Sigma(n)(n-1)a_n(z)r^n + \Sigma n\, a_n(z)r^n - \Sigma a_n(z)r^n + \Sigma a_n''(z)r^{n+2} = 0$$

$$\Sigma\,\{ n(n-1) + n - 1\}\, a_n(z)r^n = -\,\Sigma\, a_n''(z)r^{n+2}$$

For n=0, the left hand side of the last equation reduces to $-a_o(z)$, and there exists no n=1 term. Therefore,

$$-a_o(z) + \sum_{n=2}^{\infty} \{n(n-1) + n-1\} a_n(z) r^n + \sum_{n=0} a_n''(z) r^{n+2} = 0$$

$$-a_o(z) + \sum_{n=0}^{\infty} \{(n+2)(n+1)+n+1\} a_{n+2}(z) r^{n+2} + \sum_{n=0}^{\infty} a_n''(z) r^{n+2} = 0$$

$$-a_o(z) + \sum_{n=0}^{\infty} \{(n+3)(n+1)\} a_{n+2}(z) r^{n+2} + \sum_{n=0}^{\infty} a_n''(z) r^{n+2} = 0$$

$$-a_o(z) + \sum_{n=0}^{\infty} \{[(n+3)(n+1)] a_{n+2}(z) + a_n''(z)\} r^{n+2} = 0$$

The following must then be true, as for all power series expansions:

$$a_o(z) \equiv 0 \text{ , hence}$$

$$(n+3)(n+1) a_{n+2}(z) + a_n''(z) = 0$$

$$\therefore a_{n+2}(z) = \frac{-a_n''(z)}{(n+3)(n+1)}$$

Whence, a recursion relationship yields the important needed parameters. Obviously, there can be no terms for n even.

For $n = 1$ $\qquad a_3(z) = \dfrac{-a_1''(z)}{8}$

$n = 3$ $\qquad a_5(z) = \dfrac{-a_3''(z)}{24}$, etc.

$$\text{As } A(r,z) = \sum_{n=0}^{\infty} a_n(z) r^n$$

$$= a_1(z)r + a_3(z)r^3 + a_5(z)r^5 + a_7(z)r^7 + \ldots$$

Making the substitutions,

$$A = a_1(z)r - a_1''(z)\frac{r^3}{8} + \left(\frac{1}{24}\right)\left(\frac{1}{8}\right) a_1''''(z) r^5 - \ldots$$

And, to evaluate $a_1(z)$, solve for B_z using $\nabla \times A$,

$$B_z = \frac{1}{r} \cdot \frac{\partial (rA)}{\partial r} = 2a_1(z) - \frac{4}{8} a_1''(z) r^2 + \frac{6}{248} a_1''''(z) r^4 - \ldots$$

Knowing that B   is equal to $H_o(z)$ for $r = 0$, hence,

$$H_o(z) = B_z\,(r=0) = 2a_1(z), \qquad \therefore\ a_1(z) = \tfrac{1}{2} H_o(z)$$

and the expression for the Vector Potential is obtained as

$$A(r,z) = \frac{r}{2} H_o(z) - \frac{r^3}{16} H_o''(z) + \frac{r^5}{384} H_o''''(z) - \ldots \quad .$$

APPENDIX 4

THE DIFFERENTIAL EQUATION DEVELOPMENT

The essentials of this operation involve simply applying Newton's second law in cylindrical coordinates to the magnetic force acting on the particle. Finally, time and the azimuthal variables can be eliminated by means of the two motion constants, energy and the canonically conjugate angular momentum. Since the particle will begin its trajectory on the z-axis, the canonically conjugate angular momentum is, in fact, zero.

Applying Newton's 2nd law,

$$\vec{F}_{mag} = q(\vec{v} \times \vec{B}) = m(\vec{a})$$

where

$$\vec{a} \equiv \frac{d}{dt}[\vec{v}]$$

In cylindrical coordinates, the velocity vector is

$$\vec{v} = \dot{r}\,\hat{r} + r\,\dot{\phi}\,\hat{\phi} + \dot{z}\,\hat{z},$$

and, the acceleration vector is

$$\vec{a} = (\ddot{r} - r\,\dot{\phi}^2)\,\hat{r} + (2\dot{r}\,\dot{\phi} + r\,\ddot{\phi})\,\hat{\phi} + (\ddot{z})\,\hat{z}.$$

Knowing the vector potential, the magnetic field $\vec{B}$ and the quantity $\vec{v} \times \vec{B}$ can be found.

$$\vec{B} \equiv \vec{\nabla} \times \vec{A} = \frac{1}{r}\left[\frac{\partial}{\partial \phi}\left(Az\right) - \frac{\partial}{\partial z}\left(r\,A\,\phi\right)\right]\hat{r} + \left[\frac{\partial}{\partial r}\left(Az\right) - \frac{\partial}{\partial z}\left(Ar\right)\right]\hat{\phi}$$
$$+ \frac{1}{r}\left[\frac{\partial}{\partial r}\left(r\,A\,\phi\right) - \frac{\partial}{\partial \phi}\left(Ar\right)\right]\hat{z}$$

But: $\vec{A} = A_\phi\,\hat{\phi}$,

$$Ar = Az = 0$$

and,

$$\vec{B} = \frac{1}{r}\left[-\frac{\partial}{\partial z}\left(rA\,\phi\right)\right]\hat{r} + \frac{1}{r}\left[\frac{\partial}{\partial r}\left(rA\,\phi\right)\right]\hat{z}.$$

Hence:

$$\vec{v} \times \vec{B} = \left[\dot{\phi} \frac{\partial}{\partial r}\left(rA_\phi\right)\right]\hat{r} + \left[-\frac{\dot{r}}{r}\frac{\partial}{\partial r}\left(rA_\phi\right) - \frac{\dot{z}}{r}\frac{\partial}{\partial z}\left(rA_\phi\right)\right]\hat{\phi}$$

$$+ \left[\dot{\phi}\frac{\partial}{\partial z}\left(rA_\phi\right)\right]\hat{z} .$$

Equating each orthogonal cylindrical component, the following is obtained,

$$m(\ddot{r} - r\dot{\phi}^2) = q(\dot{\phi}\frac{\partial}{\partial r} rA_\phi) , \tag{4}$$

$$m(2\dot{r}\dot{\phi} + r\ddot{\phi}) = q\left[-\frac{\dot{r}}{r}\frac{\partial}{\partial r}\left(rA_\phi\right) - \frac{\dot{z}}{r}\frac{\partial}{\partial z}\left(rA_\phi\right)\right] , \tag{5}$$

$$m(\ddot{z}) = q(\dot{\phi}\frac{\partial}{\partial z} rA_\phi). \tag{6}$$

These three equations can be reduced further to:

$$\frac{d}{dt}(m\dot{r}) = mr\dot{\phi}^2 + q\dot{\phi}\frac{\partial}{\partial r}(rA_\phi),$$

$$\frac{d}{dt}(mr^2\dot{\phi} + qrA_\phi) = 0,$$

and

$$\frac{d}{dt}(m\dot{z}) = qr\dot{\phi}\frac{\partial}{\partial z}(A_\phi).$$

From the middle equation above, it can be shown that the quantity conserved is the canonically conjugate angular momentum about the symmetry axis. Thus,

$$p_c \equiv mr^2\dot{\phi} + qrA_\phi ,$$

$$\dot{\phi} = \frac{p_c - qrA_\phi}{mr^2}$$

and,

$$\frac{d}{dt}(m\dot{r}) = \frac{q^2}{m}\left[\frac{p_c}{qr} - A_\phi\right]\left[\frac{p_c}{qr^2} + \frac{\partial A_\phi}{\partial r}\right]$$

$$\frac{d}{dt}(m\dot{z}) = \frac{q^2}{m}\left[\frac{\partial A_\phi}{\partial z}\right]\left[\frac{p_c}{rq} - A_\phi\right].$$

Replacing the independent variable of time (t) with the distance on the z-axis (z) yields

$$v^2 = \left[\left(\frac{\partial r}{\partial z}\right)^2 + 1\right](\dot{z})^2 + r^2\left[\frac{p_c - qrA\,\phi}{mr^2}\right]^2 \tag{7}$$

and

$$(\dot{z})^2 = \frac{v^2 - \dfrac{q^2}{m^2}\left[\dfrac{p_c}{qr} - A\,\phi\right]^2}{\left\{1 + \left(\dfrac{dr}{dz}\right)^2\right\}}$$

This operation can be performed as follows:

$$\frac{d}{dt}(m\dot{r}) = \dot{z}\left[\frac{d}{dz}\left(m\frac{dr}{dz}\dot{z}\right)\right],$$

$$\frac{d}{dt}(m\dot{z}) = \dot{z}\left[\frac{\partial}{\partial z}(m\dot{z})\right],$$

$$\vec{v} = \dot{r}\,\hat{r} + r\,\dot{\phi}\,\hat{\phi} + \dot{z}\,\hat{z},$$

$$v^2 = \vec{v}\cdot\vec{v} = (\dot{r})^2 + (r\,\dot{\phi})^2 + (\dot{z})^2,$$

and

$$\dot{r} = \frac{dr}{dz}\dot{z},$$

$$\dot{\phi} = \frac{p_c - qrA}{mr^2}.$$

Hence:

$$v^2 = \left[\left(\frac{dr}{dz}\right)^2 + 1\right](\dot{z})^2 + r^2\left[\frac{p_c - qrA}{mr^2}\right]^2$$

$$= \left[1 + \left(\frac{dr}{dz}\right)^2\right](\dot{z})^2 + \frac{q^2}{m^2}\left[\frac{p_c}{qr} - A\right]^2.$$

Further:

$$(\dot{z})^2 = \frac{v^2 - \left(\dfrac{q}{m}\right)^2\left[\dfrac{p_c}{qr} - A\right]^2}{\left[1 + \left(\dfrac{dr}{dz}\right)^2\right]}, \tag{8}$$

and:

$$m \frac{d^2 r}{dz^2} (\dot{z})^2 + \frac{dr}{dz}\left[m\dot{z} \frac{d}{dz}(\dot{z}) \right] = \frac{q^2}{m} \left\{ \frac{p_c}{qr} - A \right\} \left[\frac{p_c}{qr^2} + \frac{\partial A}{\partial r} \right] \quad (9)$$

$$m(\dot{z}) \left[\frac{d}{dz}(z) \right] = \frac{q^2}{m} \left\{ \frac{\partial A}{\partial z} \right\} \left[\frac{p_c}{qr} - A \right] . \quad (10)$$

Combining the remaining equations 8, 9, and 10, and then allowing that

$$p_c \equiv 0$$

and

$$k \equiv \frac{mv}{q} \quad ,$$

the following equation results:

$$\frac{r''}{[1 + (r')^2]} \left\{ k^2 - A_\phi^2 \right\} - r' \left[\left(A_\phi \right) \frac{\partial A_\phi}{\partial z} \right] + \left\{ \left(A_\phi \right) \frac{\partial A_\phi}{\partial r} \right\} = 0 \quad (4\text{-}1)$$

where the dots throughout this discussion indicate derivatives with respect to time, and the primes indicate derivatives with respect to the variable z. [4]

APPENDIX 5

DEVELOPMENT OF THE VECTOR POTENTIAL

To adequately describe the field at every point, and for use in the general trajectory previously derived, equation (4-1), the following quantities are needed:

$$\vec{A} = \text{The Vector Potential},$$

$$\frac{\partial \vec{A}}{\partial z} = \text{The first partial derivative of A with respect to z},$$

and

$$\frac{\partial \vec{A}}{\partial r} = \text{The first partial derivative of A with respect to r}.$$

The vector potential, found by the power series expansion in Appendix 3, is

$$A = \frac{r}{2}[G_1] - \frac{r^3}{16}[G_2] + \frac{r^5}{384}[G_3] - \frac{r^7}{18432}[G_4] + \ldots$$

$$+ \frac{r^{13}}{29727129600}[G_7],$$

where, for the purposes of programming, the G functions are defined as follows:

$$G_1 \equiv H_0(z)$$

$$G_2 \equiv \frac{\partial^2 H_0(z)}{\partial z^2}$$

$$G_3 \equiv \frac{\partial^4 H_0}{\partial z^4}$$

$$G_5 \equiv \frac{\partial^6 H_0}{\partial z^6}$$

.

.

.

$$G_7 \equiv \frac{\partial^{12} H_0}{\partial z^{12}} \quad .$$

The first partial of $\vec{A}$ with respect to r becomes,

$$\frac{\partial \vec{A}}{\partial r} = \tfrac{1}{2}[G_1] - \frac{3r^2}{16}[G_2] + \frac{5r^4}{384}[G_3] - \frac{7r^6}{18432}[G_4] + \frac{9r^8}{1474560}[G_5]$$

$$- \frac{11r^{10}}{176047200}[G_6] + \frac{13r^{12}}{29727129600}[G_7]$$

The first partial of A with respect to z is a little more tedious, but can be shown to be,

$$\frac{\partial \vec{A}}{\partial z} = \frac{r}{2}[F_1] - \frac{r^3}{16}[F_2] + \frac{r^5}{384}[F_3] - \ldots\ldots [F_6]$$

where the F functions are defined as follows (again for programming convenience),

$$F_1 \equiv \frac{\partial G_1}{\partial z}$$

$$F_2 \equiv \frac{\partial G_2}{\partial z}$$

$$F_3 \equiv \frac{\partial G_3}{\partial z}$$

$$F_4 \equiv \frac{\partial G_4}{\partial z}$$

$$F_5 \equiv \frac{\partial G_5}{\partial z}$$

$$F_6 \equiv \frac{\partial G_6}{\partial z}$$

$$F_7 = 0.$$

APPENDIX 6

PERTINENT MACHINE PROGRAMS

The pertinent computer programs used in the solution of this problem are listed in this appendix in the following manner:

Program A - Least-squares polynomial generation by the PROGRAM CURVE, and contains 7 pages.

Program B - Theoretical off-axis field check labeled PROGRAM WATCHOUT, and contains 2 pages.

Program C - The main trajectory program labeled PROGRAM ORBITS, and contains 15 pages.

```
      PROGRAM CURVE
      DIMENSION X(18), F2(18), W(18), Y(18), DELY(18), B(18), SB(18), T(
     118), ST(18), C(18), CT(18), A(30,30)
      READ 1 (X(I),I=1,18)
    1 FORMAT (18F4.0)
      READ 200,(F2(I),I=1,18)
  200 FORMAT(12F6.4)
      CALL LSQPOL (18,12,0,0,0,SIGMA,X,F2,W,Y,DELY,B,SB,T,ST,C,CT,A)
      DO 10 I=1,18
   10 PRINT 2, I,B(I)
    2 FORMAT (15,3X,4H B =F 5.7)
      END
      SUBROUTINE LSQPOL(M,KM,IW,ISW,LP,SIGMA,X,F2,W,Y,DELY,B,SB,T,ST,C,
     1SC,A)
      DIMENSION S(30),X(1),F2(1),ST(1),SB(1),F(100),PM(100),P(100),B(1),
     1DELY(1),W(1),A(30,30),T(1),Y(1),BM(11,11),D(11,11),C(1),SC(1)
      LL=0
    9 FM=0.0
      A(1,1)=1.0
      A(2,2)=1.0
      FBAR=0.0
      XBAR=0.0
      DO10I=1,M
      IF(IW)1009,1010,1009
 1010 W2=1.0
      W(I)=1.0
      GOTO1011
 1009 W2=SQRTF(W(I))
 1011 FM=FM+W(I)
      F(I)=W2*F2(I)
      PM(I) = W2
      FBAR=FBAR+F(I)*PM(I)
   10 XBAR=XBAR+X(I)*PM(I)**2
      XBAR=XBAR/FM
      T(1)=FBAR/FM
      A(2,1)=-XBAR
```

```
      PXF=0.0
      PXP=0.0
      DO20I=1,M
      P(I)=(X(I)-XBAR)*PM(I)
      PXF=PXF+P(I)*F(I)
   20 PXP=PXP+P(I)*P(I)
      T(2)=PXF/PXP
      PMXPM=FM
      S(1)=PMXPM
      KM=KM+1
      B(1)=T(1)*A(1,1)+T(2)*A(2,1)
      B(2)=T(2)*A(2,2)
   60 DO190K=2,KM
      IF(K-2)40,165,65
   40 PRINT 4000
 4000 FORMAT(7HSTOP 40)
      STOP
   65 XPXP=0.0
      XPXPM=0.0
      B(K)=0.0
      DO70J=1,M
      XP=X(J)*P(J)
      XPXP=XPXP+XP*P(J)
   70 XPXPM=XPXPM+XP*PM(J)
      ALPHA=XPXP/PXP
      BETA=XPXPM/PMXPM
      PPXF=0.0
      PPXPP=0.0
      DO90I=1,M
   80 PT=P(I)
   81 P(I)=X(I)*PT-ALPHA*PT-BETA*PM(I)
   82 PPXF=PPXF+P(I)*F(I)
   83 PPXPP=PPXPP+P(I)*P(I)
   90 PM(I)=PT
      T(K)=PPXF/PPXPP
      PMXPM=PXP
```

```
      PXP=PPXPP
      A(K,1)=-ALPHA*A(K-1,1)-BETA*A(K-2,1)
      A(K,K-1)=A(K-1,K-2)-A(K-1,K-1)*ALPHA
      A(K,K)=1.0
      IF(K-3)150,150,110
  110 K1=K-2
      DO120I=2,K1
  120 A(K,I)=A(K-1,I-1)-ALPHA*A(K-1,I)-BETA*A(K-2,I)
  150 DO160I=1,K
  160 B(I)=B(I)+T(K)*A(K,I)
  165 SIG3=0.0
      DO180I=1,M
      Y(I)=POLYE1(X(I),K,B)
  175 DELY(I)=Y(I)-F2(I)
  180 SIG3 = SIG3 + (DELY(I)**2)*W(I)
      SIG2 = SIG3/FLOATF(M-K)
      IF(K-2)40,1650,1651
 1650 FLEV = 0.
      GO TO 1652
 1651 FLEV = (SUMDEV2 - SIG3)/SIG2
 1652 SUMDEV2 = SIG3
      SIGMA=SQRTF(SIG2)
      S(K) = PXP
      DO499I=1,K
  499 ST(I)=SIGMA/SQRTF(S(I))
      DO501I=1,K
      SB(I)=0.0
      DO500J=I,K
  500 SB(I)=SB(I)+(A(J,I)*ST(J))**2
  501 SB(I)=SQRTF(SB(I))
      IF(LP)658,183,658
  658 IF(K-2)652,651,652
  651 D(1,1)=1.0
      D(2,2)=1.0
      D(2,1)=0.0
      D(3,3)=3./2.
```

```
D(3,2)=0.
D(3,1)=-1./2.
D(4,4)=5./2.
D(4,3)=0.
D(4,2)=-3./2.
D(4,1)=0.
D(5,5)=35./8.
D(5,4)=0.
D(5,3)=-30./8.
D(5,2)=0.
D(5,1)=3./8.
D(6,6)=63./8.
D(6,5)=0.
D(6,4)=-70./8.
D(6,3)=0.
D(6,2)=15./8.
D(6,1)=0.
D(7,7)=231./16.
D(7,6)=0.
D(7,5)=-315./16.
D(7,4)=0.
D(7,3)=105./16.
D(7,2)=0.
D(7,1)=-5./16.
D(8,8)=429./16.
D(8,7)=0.
D(8,6)=-693./16.
D(8,5)=0.
D(8,4)=315./16.
D(8,3)=0.
D(8,2)=-35./16.
D(8,1)=0.
D(9,9)=6435./128.
D(9,8)=0.
D(9,7)=-12012./128.
D(9,6)=0.
```

```
      D(9,5)=6930./128.
      D(9,4)=0.
      D(9,3)=-1260./128.
      D(9,2)=0.
      D(9,1)=35./128.
      D(10,10)=12155./128.
      D(10,9)=0.
      D(10,8)=-25740./128.
      D(10,7)=0.
      D(10,6)=18018./128.
      D(10,5)=0.
      D(10,4)=-4620./128.
      D(10,3)=0.
      D(10,2)=315./128.
      D(10,1)=0.
      D(11,11)=46189./256.
      D(11,10)=0.
      D(11,9)=-109395./256.
      D(11,8)=0.
      D(11,7)=90090./256.
      D(11,6)=0.
      D(11,5)=-30030./256.
      D(11,4)=0.
      D(11,3)=3465./256.
      D(11,2)=0.
      D(11,1)=-63./256.
  652 DO700II=1,K
      J=K-II+1
      VARA=0.0
      III=K-J
      IF(III)702,701,702
  702 DO703JJ=1,III
      JK=K-JJ+1
  703 VARA=VARA+D(JK,J)*BM(K,JK)
  701 BM(K,J)=(A(K,J)-VARA)/D(J,J)
      IF(K-2)700,704,700
```

```
704 BM(1,1)=A(1,1)/D(1,1)
700 CONTINUE
705 DO708I=1,K
    C(I)=0.0
    SC(I)=0.0
    DO707J=1,K
    C(I)=C(I)+BM(J,I)*T(J)
707 SC(I)=SC(I)+(BM(J,I)*ST(J))**2
708 SC(I)=SQRTF(SC(I))
183 CONTINUE
192 PRINT 600
    PRINT 1,(I,B(I),SB(I),I=1,K)
185 PRINT 186,SIGMA,FLEV,SUMDEV2
    PRINT 601,(I,T(I),ST(I),I=1,K)
    IF(LP)187,670,187
187 PRINT 188
    PRINT 602,(I,C(I),SC(I),I=1,K)
670 PRINT 2
    PRINT 603,(I,X(I),F2(I),Y(I),DELY(I),W(I),I=1,M)
190 CONTINUE
211 IF(ISW) 210,220,210
210 DO215I=2,KM
215 PRINT 5,I,(A(I,J),J=1,I)
220 KM=KM-1
    RETURN
  1 FORMAT(3H B(0PI2,2H)=1PE15.7,6H ERRB=E10.3,3H B(0PI2,2H)=1PE15.7,
   16H ERRB=E10.3,3H B(0PI2,2H)=1PE15.7,6H ERRB=E10.3)
  2 FORMAT(4H0   I 11X 4HX(I) 12X4HF(I)12X4HY(I)12X7HDELY(I)10X4HW(I)/)
  5 FORMAT(36H0 ORTHOGONAL POLYNOMIAL COEFF FOR K=I5//(1P8E15.6))
186 FORMAT(7H0SIGMA=1PE16.7,9H F LEVEL=1PE16.7,12H SUM SQ DEV=,1PE16.7
   *                         //  45H COEFFICIENTS OF Y=T1*P1+T2*P2+ETC AND
   1 ERRORS/)
188 FORMAT(23H0  LEGENDRE POLYNOMIALS/45H COEFFICIENTS OF Y=C1*L1+C2*L
   12+ETC AND ERRORS/)
600 FORMAT(41H1COEFFICIENTS OF Y=B1+B2*X+ETC AND ERRORS/)
601 FORMAT(3H T(I2,2H)=1PE15.7,6H ERRT=E10.3,3H T(0PI2,2H)=1PE15.7,6H
```

```
     1ERRT=E10.3,3H T(0PI2,2H)=1PE15.7,6H ERRT=E10.3)
  602 FORMAT(3H C(I2,2H)=1PE15.7,6H ERRC=E10.3,3H C(0PI2,2H)=1PE15.7,6H
     1ERRC=E10.3,3H C(0PI2,2H)=1PE15.7,6H ERRC=E10.3)
  603 FORMAT(I6,1P5E16.7)
      END
      FUNCTION POLYE1(X,K,B)
      DIMENSION B(30)
   10 S=B(K)
      KK=K-1
   20 DO 40 I=1,KK
   30 IK=K-I
   40 S=X*S+B(IK)
      POLYE1=S
       END
      END

.00 .02 .06 .10 .14 .18 .22 .26 .30 .34 .38 .42 .46 .50 .54 .58 .62 .66
  805    793    702    566    428    313    230    172    131    100     80     64
   53     43     36     31     26     24
```

```
      PROGRAM WATCHOUT
      DIMENSION G(20),B(20),ZZ(20),RR(20),H(20,20)
      B( 1)=  8.0498907E-02
      B( 2)=  2.3351831E-02
      B( 3)= -4.8664438E+00
      B( 4)=  4.2887590E+01
      B( 5)= -4.3626183E+02
      B( 6)=  3.9271101E+03
      B( 7)= -2.2648265E+04
      B( 8)=  8.2393030E+04
      B( 9)= -1.9359723E+05
      B(10)=  2.9437706E+05
      B(11)= -2.8025472E+05
      B(12)=  1.5200646E+05
      B(13)= -3.5865075E+04
      ZZ(1)=-0.00
      ZZ(2)=-0.14
      RR(1)=.0
      RR(2)=0.0127
      RR(3)=0.0254
      RR(4)=0.0381
      RR(5)=0.0508
      RR(6)=0.0635
      RR(7)=0.0762
      DO 10 I=1,3
      Z=ZZ(I)
      G(1)=B(1)+B(2)*Z+B(3)*Z**2+B(4)*Z**3+B(5)*Z**4+B(6)*Z**5+B(7)*Z**6
     1+B(8)*Z**7+B(9)*Z**8+B(10)*Z**9+B(11)*Z**10+B(12)*Z**11+B(13)*Z**1
     22
      G(2)=2.*B(3)+6.*B(4)*Z+12.*B(5)*Z**2+20.*B(6)*Z**3+30.*B(7)*Z**4+4
     12.*B(8)*Z**5+56.*B(9)*Z**6+72.*B(10)*Z**7+90.*B(11)*Z**8+110.*B(12
     2)*Z**9+132.*B(13)*Z**10
      G(3)=24.*B(5)+120.*B(6)*Z+360.*B(7)*Z**2+840.*B(8)*Z**3+1680.*B(9)
     1*Z**4+3024.*B(10)*Z**5+5040.*B(11)*Z**6+7920.*B(12)*Z**7+11880.*B(
     213)*Z**8
      G(4)=720.*B(7)+5040.*B(8)*Z+20160.*B(9)*Z**2+60480.*B(10)*Z**3+151
```

```
     1200.*B(11)*Z**4+332640.*B(12)*Z**5+665280.*B(13)*Z**6
      G(5)=40320.*B(9)+362880.*B(10)*Z+1814400.*B(11)*Z**2+6652800.*B(12
     1)*Z**3+19958400.*B(13)*Z**4
      G(6)=3628800.*B(11)+39916800.*B(12)*Z+239500800.*B(13)*Z**2
      G(7)=479001600.*B(13)
      PRINT 30, (G(KK),KK=1,7)
      DO 10 J=1,7
      R=RR(J)
      H(I,J)=G(1)-G(2)*R**2/4.+G(3)*R**4/64.-G(4)*R**6/2304.+G(5)*R**8/1
     147456.-G(6)*R**10/14745600.+G(7)*R**12/2123366400.
   10 CONTINUE
      PRINT 20,(ZZ(I),I=1,3)
   20 FORMAT (1H1///,15X,7E15.8)
      DO 40 J=1,7
      PRINT 30,RR(J),(H(I,J),I=1,3)
   30 FORMAT (//8E15.8)
   40 CONTINUE
      END
      END
```

```
      PROGRAM ORBITS
      DIMENSION X(30),XDOT(30),C(15),B(15),F(15),G(15)
      C(10)=1
    1 CALL INTEG1(T,X,XDOT,C)
C     ENER=ENERGY OF THE H2 ION IN ELECTRON-VOLTS
      ENER=C(1)
C     OKAY=(MOM/CHARGE)*(MOM/CHARGE)
      OKAY=(4.17576E-08)*(ENER)
C     P IS THE DECIMAL FRACTION OF THE MAG FLD CURRENT DESIRED
      P=C(2)
      B( 1)=  8.0498907E-02
      B( 2)=  2.3351831E-02
      B( 3)= -4.8664438E+00
      B( 4)=  4.2887590E+01
      B( 5)= -4.3626183E+02
      B( 6)=  3.9271101E+03
      B( 7)= -2.2648265E+04
      B( 8)=  8.2393030E+04
      B( 9)= -1.9359723E+05
      B(10)=  2.9437706E+05
      B(11)= -2.8025472E+05
      B(12)=  1.5200646E+05
      B(13)= -3.5865075E+04
      F(1)=B(2)+2.*B(3)*T+3.*B(4)*T**2+4.*B(5)*T**3+5.*B(6)*T**4+6.*B(7)
     1*T**5+7.*B(8)*T**6+8.*B(9)*T**7+9.*B(10)*T**8+10.*B(11)*T**9+11.*B
     2(12)*T**10+12.*B(13)*T**11
      F(2)=6.*B(4)+24.*B(5)*T+60.*B(6)*T**2+120.*B(7)*T**3+210.*B(8)*T**
     14+336.*B(9)*T**5+504.*B(10)*T**6+720.*B(11)*T**7+990.*B(12)*T**8+1
     2320.*B(13)*T**9
      F(3)=120.*B(6)+720.*B(7)*T+2520.*B(8)*T**2+6720.*B(9)*T**3+15120.*
     1B(10)*T**4+30240.*B(11)*T**5+55440.*B(12)*T**6+95040.*B(13)*T**7
      F(4)=5040.*B(8)+40320.*B(9)*T+181440.*B(10)*T**2+604800.*B(11)*T**
     13+1663200.*B(12)*T**4+3991680.*B(13)*T**5
      F(5)=362880.*B(10)+3628800.*B(11)*T+19958400.*B(12)*T**2+79833600.
     1*B(13)*T**3
      F(6)=39916800.*B(12)+479001600.*B(13)*T
```

```
      VECDZ=X(1)*F(1)/2.-F(2)*X(1)**3/16.+F(3)*X(1)**5/384.-F(4)*X(1)**7
     1/18432.+F(5)*X(1)**9/1474560.-F(6)*X(1)**11/176947200.
      G(1)=B(1)+B(2)*T+B(3)*T**2+B(4)*T**3+B(5)*T**4+B(6)*T**5+B(7)*T**6
     1+B(8)*T**7+B(9)*T**8+B(10)*T**9+B(11)*T**10+B(12)*T**11+B(13)*T**1
     22
      G(2)=2.*B(3)+6.*B(4)*T+12.*B(5)*T**2+20.*B(6)*T**3+30.*B(7)*T**4+4
     12.*B(8)*T**5+56.*B(9)*T**6+72.*B(10)*T**7+90.*B(11)*T**8+110.*B(12
     2)*T**9+132.*B(13)*T**10
      G(3)=24.*B(5)+120.*B(6)*T+360.*B(7)*T**2+840.*B(8)*T**3+1680.*B(9)
     1*T**4+3024.*B(10)*T**5+5040.*B(11)*T**6+7920.*B(12)*T**7+11880.*B(
     213)*T**8
      G(4)=720.*B(7)+5040.*B(8)*T+20160.*B(9)*T**2+60480.*B(10)*T**3+151
     1200.*B(11)*T**4+332640.*B(12)*T**5+665280.*B(13)*T**6
      G(5)=40320.*B(9)+362880.*B(10)*T+1814400.*B(11)*T**2+6652800.*B(12
     1)*T**3+19958400.*B(13)*T**4
      G(6)=3628800.*B(11)+39916800.*B(12)*T+239500800.*B(13)*T**2
      G(7)=479001600.*B(13)
      VECDR=G(1)/2.-3.*G(2)*X(1)**2/16.+5.*G(3)*X(1)**4/384.-7.*G(4)*X(1
     1)**6/18432.+9.*G(5)*X(1)**8/1474560.-11.*G(6)*X(1)**10/176947200.+
     213.*G(7)*X(1)**12/29727129600.
      VECPT=X(1)*G(1)/2.-G(2)*X(1)**3/16.+G(3)*X(1)**5/384.-G(4)*X(1)**7
     1/18432.+G(5)*X(1)**9/1474560.-G(6)*X(1)**11/176947200.+G(7)*X(1)**
     213/29727129600.
      FUNC1=OKAY-VECPT*VECPT*P*P
      FUNC2=VECPT*VECDZ*P*P
      FUNC3=VECPT*VECDR*P*P
      FUNC4=(FUNC2)/(FUNC1)
      FUNC5=(FUNC3)/(FUNC1)
      XDOT(2)=X(2)*(FUNC4)+X(2)*X(2)*X(2)*(FUNC4)-X(2)*X(2)*(FUNC5)-(FUN
     1C5)
      XDOT(1)=X(2)
      GO TO 1
      END
      SUBROUTINE INTEG1 (TC, XC, DX, C)                                 00000000
*                                                                       0      10
C          SUBROUTINE USES FOURTH-ORDER RUNGE-KUTTA METHOD TO INTEGRATE 00000020
```

```
C          ORDINARY DIFFERENTIAL EQUATIONS SUPPLIED BY THE CALLING
C          PROGRAM. SINCE THESE EQUATIONS MUST BE REPEATEDLY QUOTE
C          CALLED UNQUOTE BY THIS PROGRAM, A COMPUTED GO TO IS HERE
C          USED TO ENSURE RETURN TO THE CORRECT PART OF THIS SUBROUTINE.
*
C         COMPLETED NOVEMBER 1963
C          REVISED JUNE 1964 AND JUNE 1965
      DIMENSION X(30), DX(30), C(15), XC(30), ITITLE(12), JTITLE(10),
     1          KTITLE(10), X1(900), X2(900), X3(900), X4(900),
     2          Y1(900), Y2(900), Y3(900), Y4(900), IP(10), IG(10),
     3          PR(10), GR(10) ,TX(6), TY(6)
      INDIC = C(10)
      GO TO (1, 2000, 50, 58, 88, 88),INDIC
*
C          READ DATA AND PRINT RECORD.
*
    1 READ 100, (ITITLE(I), I=1,6 )
      READ 101,NR
      READ 102, NN
      NRC = 0
      IF(NN- 30)1000,1000,2
    2 PRINT 200
      STOP
 1000 NRC = NRC + 1
      PRINT 201, (ITITLE(I), I=1,6)
      IF (NRC - 1)6,3,6
    3 IF (NR - 1)4,5,4
    4 PRINT 202, NR
      GO TO 6
    5 PRINT 203
      GO TO 7
    6 PRINT 204, NRC
    7 PRINT 205, NN
  100 FORMAT (10A8)
  101 FORMAT (I1)
  102 FORMAT (I2)
```

```
200 FORMAT (////,48H ERROR IN ORDER OF EQUATION. MUST NOT EXCEED 30. )
201 FORMAT (1H1,/////,36X,6A8)
202 FORMAT (/,37X,I1,20H RUNS ARE CALLED FOR )
203 FORMAT (/,37X,21HONE RUN IS CALLED FOR ,///,18H INPUT DATA RECORD)
204 FORMAT (///,34H INPUT DATA RECORD FOR RUN NUMBER  ,I1)
205 FORMAT (//,22H ORDER OF EQUATIONS = ,I2)
    READ 103, TI, DT, TF1, DT2, TF2, DT3, TF3
103 FORMAT (8F10.4)
    IF(DT2)9,8,9
  8 TF = TF1
    PRINT 206, TI, TF
    PRINT 207,DT
206 FORMAT (22H INITIAL TIME        = ,E10.4,/
  1         22H FINAL TIME          = ,E10.4)
207 FORMAT (22H STEP SIZE           = ,E10.4)
    GO TO 12
  9 IF(DT3)11,10,11
 10 TF = TF2
    PRINT 206, TI, TF
    PRINT 208, DT, TI, TF1, DT2, TF1, TF
208 FORMAT (22H STEP SIZE           = ,E10.4,13H BETWEEN T = ,E10.4,
  1          9H AND T = ,E10.4)
    GO TO 12
 11 TF = TF3
    PRINT 206, TI, TF
    PRINT 208, DT, TI, TF1, DT2, TF1, TF2, DT3, TF2, TF
 12 READ 103, (C(I), I=1,8)
    READ 103, (X(I), I=1,NN)
    J = 0
    DO 14 I=1,8
    IF(C(I))13,14,13
 13 J = J + 1
 14 CONTINUE
    K = 0
    DO 16 I=1,NN
    IF(X(I))15,16,15
```

```
   15 K = K + 1
   16 CONTINUE
      IF(J - 1)17,18,19
   17 PRINT 209
      GO TO 423
   18 PRINT 210
      GO TO 420
   19 PRINT 211
  420 DO 422 I=1,8
      IF(C(I))421,422,421
  421 PRINT 212, I, C(I)
  422 CONTINUE
  209 FORMAT (/,34H ALL THE CONSTANTS, C(I), ARE ZERO )
  210 FORMAT (/,30H THE ONLY NON-ZERO CONSTANT IS )
  211 FORMAT (/,35H THE NON-ZERO CONSTANTS, C(I), ARE )
  212 FORMAT (14X,2HC(,I2,4H) = ,E10.4)
  423 IF(K - 1)424,425,426
  424 PRINT 1209
      GO TO 20
  425 PRINT 1210
      GO TO 427
  426 PRINT 1211
  427 DO 429 I=1,NN
      IF(X(I))428,429,428
  428 PRINT 1212, I, X(I)
  429 CONTINUE
 1209 FORMAT (/,36H ALL THE INITIAL CONDITIONS ARE ZERO )
 1210 FORMAT (/,39H THE ONLY NON-ZERO INITIAL CONDITION IS )
 1211 FORMAT (/,36H THE NON-ZERO INITIAL CONDITIONS ARE )
 1212 FORMAT (14X,2HX(,I2,4H) = ,E10.4)
   20 READ 104, (JTITLE(I), IP(I), I = 1,8)
  104 FORMAT(8(A8,I2))
*
C     CHECK FOR THE NUMBER OF COLUMNS CALLED FOR BY LOCATING FIRST
C     BLANK COLUMN HEADING
*
```

```
      IBLANK = 8H
      DO 21 J=1,8
      IF(JTITLE(J) - IBLANK)21,22,21
   21 CONTINUE
      J = 9
   22 JJ = J - 1
*
C     JJ IS NOW THE NUMBER OF COLUMNS. REPEAT WITH THE GRAPHS.
*
      READ 105, (KTITLE(I), KTITLE(I+1), IG(I), IG(I+1), I=1,7,2)
  105 FORMAT (4(2A8,2I2))
      DO 24 K=1,7,2
      IF(KTITLE(K) - IBLANK)24,23,24
   23 IF(KTITLE(K+1) - IBLANK)24,25,24
   24 CONTINUE
      K = 8
   25 KK = K/2
      KKK = KK*2
      MULTIP = 0
      IF(KK -1)306,300,306
  300 IF(IG(3) + IG(4))301,306,301
  301 IF(IG(5) + IG(6))303,302,303
  302 MULTIP = 2
      KKK = 4
      GO TO 306
  303 IF(IG(7) + IG(8))305,304,305
  304 MULTIP = 3
      KKK = 6
      GO TO 306
  305 MULTIP = 4
      KKK = 8
*
C     IF MULTIP = 0, KK IS THE NUMBER OF SINGLE CURVE GRAPHS. OTHERWISE
C     MULTIP IS THE NUMBER OF CURVES ON A SINGLE GRAPH.
*
  306 IF(JJ)26,27,26
```

```
   26 PRINT 214, (JTITLE(I), IP(I), I=1,JJ)
  214 FORMAT (///,56H THE COLUMN HEADINGS AND THE CORRESPONDING VARIABLE
     1S ARE ,//,(10X,A8,4X,2HX(,I2,1H)))
      GO TO 28
   27 PRINT 215
  215 FORMAT (///,25H NO PRINTOUT IS REQUIRED  )
   28 IF(KK)29,308,29
   29 IF(MULTIP)309,30,309
   30 IF(KK - 1)307,1306,307
 1306 PRINT 216, KTITLE(1), KTITLE(2), IG(1), IG(2)
  216 FORMAT (///,52H THE GRAPH TITLE AND THE CORRESPONDING VARIABLES AR
     1E ,//,10X,2A8,4X,2HX(,I2,8H) VS. X(,I2,1H))
      GO TO 31
  307 PRINT 217, (KTITLE(I), KTITLE(I+1), IG(I), IG(I+1), I=1,KKK ,2)
  217 FORMAT (///,64H THE INDIVIDUAL GRAPH TITLES AND THE CORRESPONDING
     1VARIABLES ARE ,//,(10X,2A8,4X,2HX(,I2,8H) VS. X(,I2,1H)))
      GO TO 31
  308 PRINT 1217
 1217 FORMAT(///,24H NO GRAPHS ARE REQUIRED  )
      GO TO 31
  309 PRINT 1220
 1220 FORMAT (///,52H THE GRAPH TITLE AND THE CORRESPONDING VARIABLES AR
     1E ,/)
      PRINT 1221, KTITLE(1), KTITLE(2), (IG(I), IG(I+1), I=1,KKK,2)
 1221 FORMAT (10X,2A8,4X,2HX(,I2,8H) VS. X(,I2,1H),/, (30X,2HX(,I2,
     1        8H) VS. X(,I2,1H)))
*
C     THIS ENDS THE BOOK-KEEPING. INITIALIZE BEFORE ENTERING MAIN LOOP.
*
   31 IPAGE = 0
      T = TI
      NOPTS = 0
      NUMPTS = 0
      ITITLE(8) = 8H
      ITITLE(11)= 8H
      ITITLE(12)= 8H
```

```
      GO TO (32,33,34,35,36,37,38,39,40),NRC
   32 ITITLE(7) = 8H RUN 1
      GO TO 41
   33 ITITLE(7) = 8H RUN 2
      GO TO 41
   34 ITITLE(7) = 8H RUN 3
      GO TO 41
   35 ITITLE(7) = 8H RUN 4
      GO TO 41
   36 ITITLE(7) = 8H RUN 5
      GO TO 41
   37 ITITLE(7) = 8H RUN 6
      GO TO 41
   38 ITITLE(7) = 8H RUN 7
      GO TO 41
   39 ITITLE(7) = 8H RUN 8
      GO TO 41
   40 ITITLE(7) = 8H RUN 9
   41 C(11) = 20.
      C(12) = 5.
      C(13) = DT
      DO 42 I=1,NN
   42 XC(I) = X(I)
      TC = T
      C(10) = 2.
      RETURN
 2000 IF(JJ)43,54,43
   43 INCPR = C(11)
      C(11) = 20.
      IF(XMODF(NOPTS,50*INCPR))44,46,44
   44 IF(XMODF(NOPTS,10*INCPR))45,47,45
   45 IF(XMODF(NOPTS,    INCPR))54,48,54
   46 IPAGE = IPAGE + 1
      IF(NR - 1)1046,1047,1046
 1046 PRINT 218, (ITITLE(I), I=1,6), IPAGE, ITITLE(7), (JTITLE(I),I=1,8)
      PRINT 219
```

```
      GO TO 47
 1047 PRINT 1218, (ITITLE(I), I=1,6), IPAGE, (JTITLE(I), I=1,8)
      PRINT 219
   47 PRINT 219
  218 FORMAT (1H1,///,20X,6A8,10X,5HPAGE ,I1,14H OF OUTPUT FOR,A8,/////,
     1        11X,8(A8,5X))
 1218 FORMAT (1H1,///,20X,6A8,30X,5HPAGE ,I1,/////,11X,8(A8,5X))
  219 FORMAT (1H  )
   48 DO 49 I=1,NN
   49 XC(I) = X(I)
      TC = T
      C(10) = 3.
      RETURN
   50 DO 53 I=1,JJ
      IF(IP(I))52,51,52
   51 PR(I) = T
      GO TO 53
   52 IPI = IP(I)
      PR(I) = XC(IPI)
   53 CONTINUE
      PRINT 220, (PR(I), I=1,JJ)
  220 FORMAT (7X, 8E13.5)
   54 IF(KK)55,62,55
   55 INCGR = C(12)
      C(12) = 5.
      IF(XMODF(NOPTS, INCGR))62,56,62
   56 DO 57 I=1,NN
   57 XC(I) = X(I)
      TC = T
      C(10) = 4.
      RETURN
   58 DO 61 I=1,KKK
      IF(IG(I))60,59,60
   59 GR(I) = T
      GO TO 61
   60 IGI = IG(I)
```

```
      GR(I) = XC(IGI)
   61 CONTINUE
      IF(KKK - 8)1611,1610,1610
 1611 KP1 = KKK + 1
      DO 1612 I=KP1,8
 1612 GR(I) = 0.
 1610 NUMPTS = NUMPTS + 1
      Y1(NUMPTS) = GR(1)
      X1(NUMPTS) = GR(2)
      Y2(NUMPTS) = GR(3)
      X2(NUMPTS) = GR(4)
      Y3(NUMPTS) = GR(5)
      X3(NUMPTS) = GR(6)
      Y4(NUMPTS) = GR(7)
      X4(NUMPTS) = GR(8)
   62 NOPTS = NOPTS + 1
      IF(NUMPTS - 900)64,63,64
   63 PRINT 221
  221 FORMAT (//////,25H STOP AT 900 GRAPH POINTS    )
      GO TO 91
   64 IF(NOPTS - 4500)66,65,66
   65 PRINT 222
  222 FORMAT (//////,31H STOP AT 4500 INTEGRATION STEPS   )
      GO TO 91
   66 IF(IPAGE - 9)69,67,68
   67 IF(XMODF(NOPTS , 50*INCPR))69,68,69
   68 PRINT 223
  223 FORMAT (//////,27H STOP AT 9 PAGES OF OUTPUT   )
      GO TO 91
   69 DO 70 I=1,NN
      IF(ABSF(X(I)) - 1.0E+12)70,70,71
   70 CONTINUE
      GO TO 72
   71 PRINT 224
  224 FORMAT (//////,76H STOP WITH THE ABSOLUTE VALUE OF A DEPENDENT VAR
     1IABLE GREATER THAN 1.0E+12.  ,/,57H INTEGRATION PROBABLY UNSTABLE.
```

```
    2 TRY A SMALLER STEP SIZE. ,26HNO GRAPHS WILL BE PLOTTED.        )  00002910
      GO TO 330                                                         00002920
   72 DT = C(13)                                                        00002930
      IF(TI - TF)73,73,80                                               00002940
   73 IF(T - TF)75,74,74                                                00002950
   74 PRINT 225                                                         00002960
  225 FORMAT (//////,26H NORMAL STOP AT FINAL TIME    )                 00002970
      GO TO 91                                                          00002980
   75 IF(T - TF1)76,77,77                                               00002990
   76 C(13) = DT                                                        00003000
      GO TO 87                                                          00003010
   77 IF(T - TF2)78,79,79                                               00003020
   78 C(13) = DT2                                                       00003030
      GO TO 87                                                          00003040
   79 C(13) = DT3                                                       00003050
      GO TO 87                                                          00003060
   80 IF(TF - T)82,74,74                                                00003070
   82 IF(TF1 - T)76,84,84                                               00003080
   84 IF(TF2 - T)78,79,79                                               00003090
   87 C(10) = 5.                                                        00003100
   88 CALL RKUTTA2(NN, T, X, DT, C, TC, XC, DX)                         00003110
      IF(C(10) - 6.)90,89,90                                            00003120
   89 RETURN                                                            00003130
   90 T = T + DT                                                        00003140
      GO TO 2000                                                        00003150
   91 IF(KK)92,330,92                                                   00003160
   92 IF(MULTIP)97,93,97                                                00003170
   93 LABEL = 4H                                                        00003180
      ITITLE(9) = KTITLE(1)                                             00003190
      ITITLE(10)= KTITLE(2)                                             00003200
      CALL DRAW (NUMPTS,Y1,X1,0,0,LABEL,ITITLE,0.04,0.04,0,0,2,2,8,15,1,00003211
     1           LAST)                                                  00003212
      IF(KK - 1)94,330,94                                               00003220
   94 ITITLE(9) = KTITLE(3)                                             00003230
      ITITLE(10)= KTITLE(4)                                             00003240
      CALL DRAW (NUMPTS,Y2,X2,0,0,LABEL,ITITLE,0.04,0.04,0,0,2,2,8,15,1,00003251
```

```
     1              LAST)
      IF(KK - 2)95,330,95
   95 ITITLE(9) = KTITLE(5)
      ITITLE(10)= KTITLE(6)
      CALL DRAW (NUMPTS,Y3,X3,0,0,LABEL,ITITLE,0.04,0.04,0,0,2,2,8,15,1,
     1              LAST)
      IF(KK - 3)96,330,96
   96 ITITLE(9) = KTITLE(7)
      ITITLE(10)= KTITLE(8)
      CALL DRAW (NUMPTS,Y4,X4,0,0,LABEL,ITITLE,0.04,0.04,0,0,2,2,8,15,1,
     1              LAST)
      GO TO 330
*
C     NOW PLOT DUMMY CURVE ALONG AXES TO SET SCALES.
*
   97 BIGX = 0.
      BIGY = 0.
      SMLX = 0.
      SMLY = 0.
      DO 1970 I=1,NUMPTS
      XMAX = MAX1F ( X1(I), X2(I), X3(I), X4(I))
      YMAX = MAX1F ( Y1(I), Y2(I), Y3(I), Y4(I))
      XMIN = MIN1F (X1(I), X2(I), X3(I), X4(I))
      YMIN = MIN1F( Y1(I), Y2(I), Y3(I), Y4(I))
      IF (BIGX - XMAX) 1971,1972,1972
 1971 BIGX = XMAX
 1972 IF (BIGY-YMAX)1973,1974,1974
 1973 BIGY = YMAX
 1974 IF (SMLX - XMIN) 1976,1976,1975
 1975 SMLX = XMIN
 1976 IF (SMLY - YMIN)1970,1970,1977
 1977 SMLY = YMIN
 1970 CONTINUE
      TX(1) = 0.
      TX(2) = 0.
      TX(3) = 0.
```

```
      TX(4) = SMLX
      TX(5) = BIGX
      TY(1) = BIGY
      TY(2) = SMLY
      TY(3) = 0.
      TY(4) = 0.
      TY(5) = 0.
      LABEL = 4H
      ITITLE(9) = KTITLE(1)
      ITITLE(10)= KTITLE(2)
      CALL DRAW (5,TX,TY,1,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,1,LAST)
      MODCURV = 2
      LABEL = 4H 1
      CALL DRAW (NUMPTS,X1,Y1,MODCURV,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,
     1           0,LAST)
      IF(MULTIP - 2)98,98,99
   98 MODCURV = 3
      GO TO 325
   99 MODCURV = 2
  325 LABEL = 4H 2
      CALL DRAW (NUMPTS,X2,Y2,MODCURV,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,
     1           0,LAST)
      IF(MULTIP - 3)330,326,327
  326 MODCURV = 3
      GO TO 328
  327 MODCURV = 2
  328 LABEL = 4H 3
      CALL DRAW (NUMPTS,X3,Y3,MODCURV,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,
     1           0,LAST)
      IF(MULTIP - 4)330,329,329
  329 MODCURV = 3
      LABEL = 4H 4
      CALL DRAW (NUMPTS,X4,Y4,MODCURV,0,LABEL,ITITLE,.1,.01,0,0,2,0,0,0,
     1           0,LAST)
  330 IF(NRC - NR)1000,331,1000
  331 IF(NR - 1)333,332,333
```

```
332 PRINT 226
    STOP
333 PRINT 227, NR
    STOP
226 FORMAT(//,43H THE ONE RUN CALLED FOR HAS BEEN COMPLETED. ,//)
227 FORMAT(//,5H THE ,I1,37H RUNS CALLED FOR HAVE BEEN COMPLETED.,//)
    END
    SUBROUTINE RKUTTA2(NN, T, X, DT, C, TC, XC, DX)
    DIMENSION X(30), C(15), XC(30), DX(30), CT(4), AK(4,30)
    INDIC = C(10) - 4.0
    GO TO (1, 3),INDIC
  1 CT(1) = 0.0
    CT(2) = 0.5
    CT(3) = 0.5
    CT(4) = 1.0
    DO 4 II=1,4
    TC = T + CT(II)*DT
    DO 2 J=1,NN
  2 XC(J) = X(J) + CT(II)*AK(II-1, J)
    C(10) = 6.0
    RETURN
  3 DO 4 J=1,NN
  4 AK(II, J) = DT*DX(J)
    DO 5 J=1,NN
  5 X(J) =X(J) + (AK(1,J) + 2.*AK(2,J) + 2.*AK(3,J) + AK(4,J))/6.0
    C(10) = 7.0
    RETURN
    END
    END
```

Typical Input Data

Note: The data cards are in the same order as their explanation

```
 GAGLIANO, ROSS A.  TRAJECTORIES
1
 2
    .00   0.005      0.06       0.0005   0.1600    0.005      0.5000
    300.0  1.20
     .00  1.000
Z DIST   00RADIUS  01SLOPE    02
    45.00        0100
```

Typical Output Data

GAGLIANO, RCSS A. TRAJECTORIES

Z DIST	RADIUS	SLOPE
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]

[illegible]

GRAPH TITLE . . [illegible] TRAJECTORIES

[illegible].

STOP

TIME, 2 [illegible] SECONDS

APPENDIX 7

GRAPHS OF VARIOUS TRAJECTORIES

This appendix contains these four figures which show trajectories as produced by PROGRAM ORBITS.

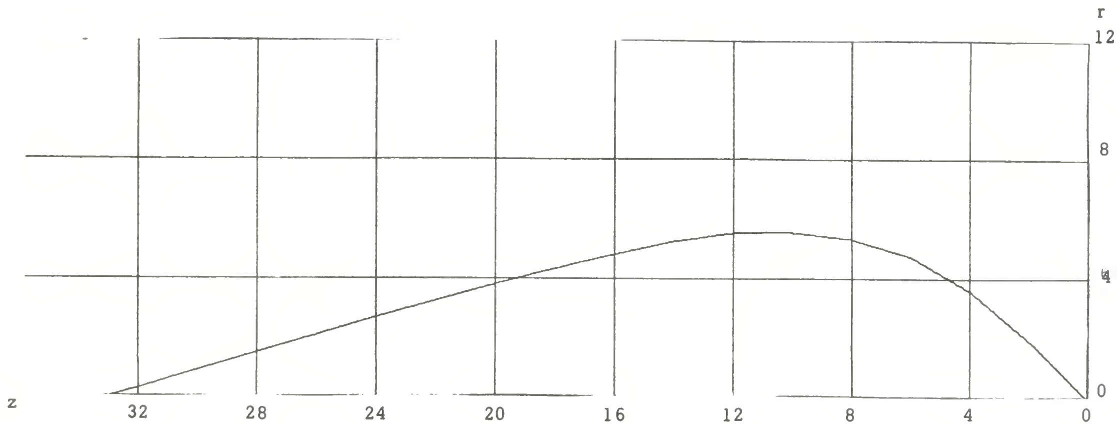

Fig. 3. The Standard Trajectory

The energy E_o = 300 eV, and the magnetization current is 12 amps. The scattering (initial) angle is 45^o.

NOTE: From the origin in the lower right hand corner, the radial distance (r) is plotted versus the axial distance (z), and both are in centimeters. Further, z is positive to the left.

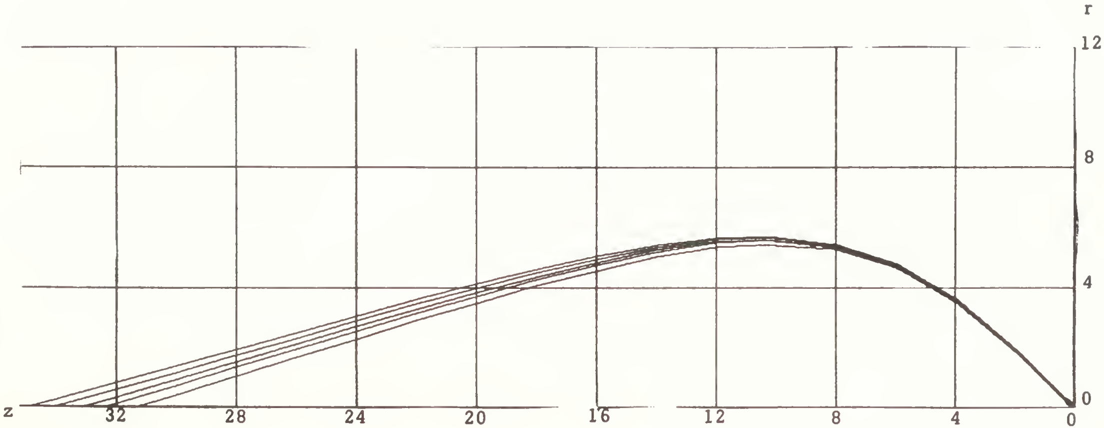

Fig. 4. Trajectories showing variation in energy

The field and initial angle were held constant, magnetization current of 12 amps and $\Theta = 45^{\circ}$.

The energy E_o was varied as follows: 300 ± 5 eV and 300 ± 10 eV.

The above curves range from 290 eV (the lowest curve) to 310 eV (the highest).

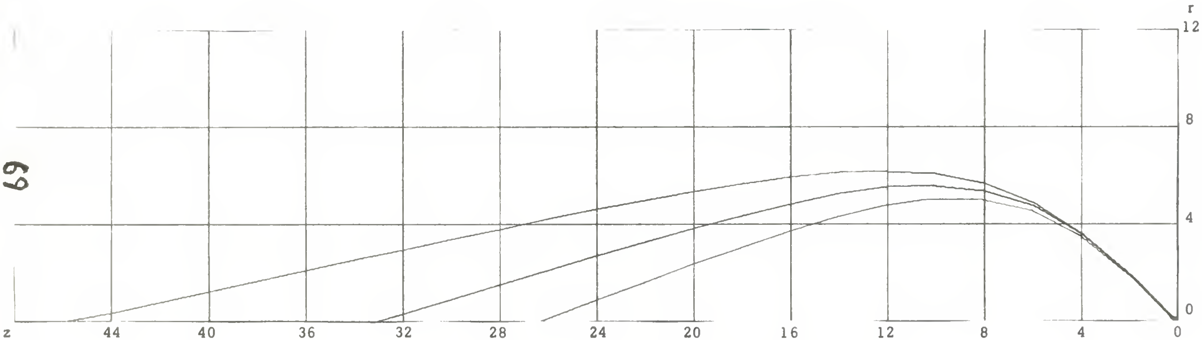

Fig. 5. Trajectories showing variation in magnetic field
The magnetizing current has values of 11, 12 and 13 amps.
E_o = 300 eV and $\Theta = 45^o$, and both were held constant.

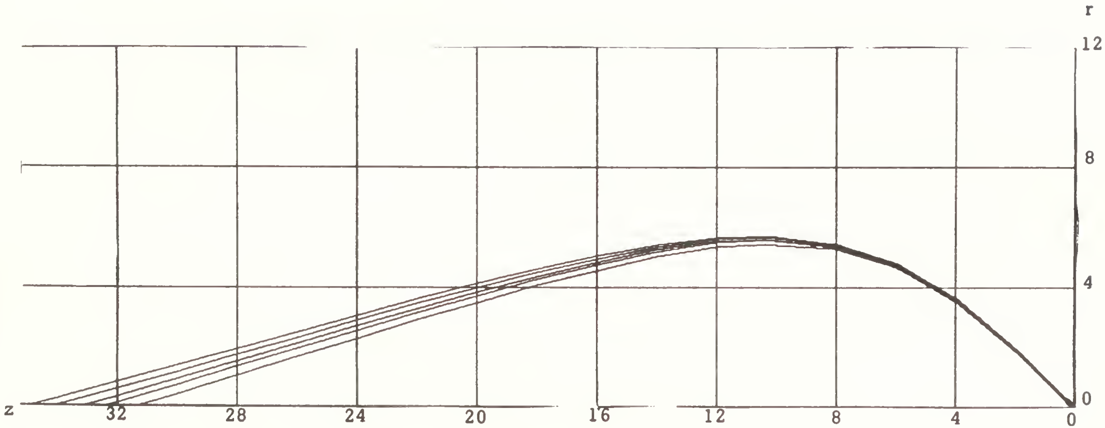

Fig. 4. Trajectories showing variation in energy

The field and initial angle were held constant, magnetization current of 12 amps and $\Theta = 45^{\circ}$.

The energy E_o was varied as follows: 300 $\pm$ 5 eV and 300 $\pm$ 10 eV.

The above curves range from 290 eV (the lowest curve) to 310 eV (the highest).

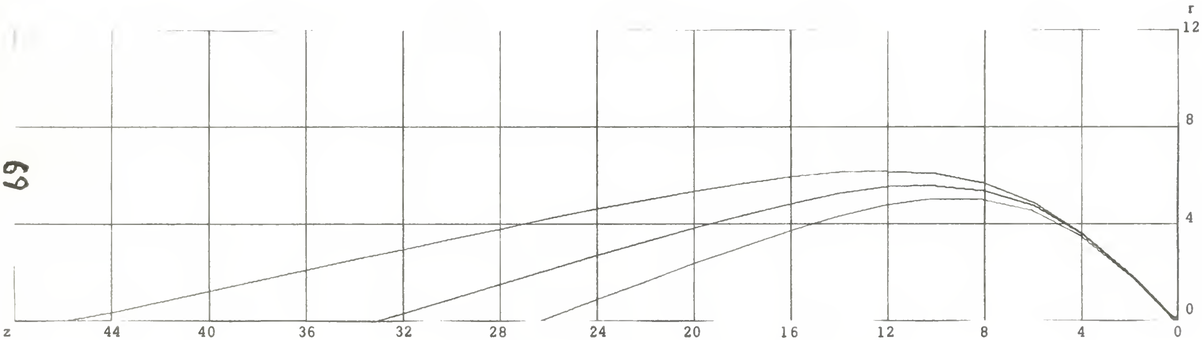

Fig. 5. Trajectories showing variation in magnetic field
The magnetizing current has values of 11, 12 and 13 amps.
E_O = 300 eV and $\Theta = 45^{o}$, and both were held constant.

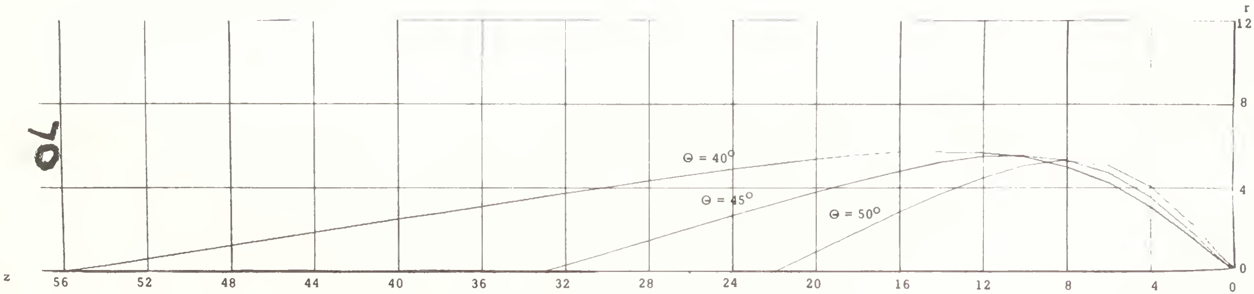

Fig. 6. Trajectories showing variation in initial angle, where Θ is varied as shown above. E_o = 300 eV and the magnetization current = 12 amps.

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This theoretical study of the trajectories of charged particles supplements an experimental project of molecular-ionic rearrangements using the magnetic focusing properties of a beta-ray spectrometer. The experimentally measured magnetic field was analytically represented by a twelfth-order polynomial. This field is axially symmetric, but non-homogeneous otherwise. The particular particle of concern was the hydrogen ion, H_2^+. The trajectory of this particle was computed from a second-order differential equation, assuming values for the kinetic energy and initial angle of the particle, and the magnetizing current. The solution was obtained by numerical integration using a CDC 1604 digital computer. The distinctive feature of these calculations, in contrast to those used normally for a beta-ray spectrometer, is the large scattering (initial) angle, about 45°.

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